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SciDAC-3

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# ComPASS

## Advanced Computation for HEP Accelerator Science and Technology

Panagiotis Spentzouris (Fermilab)  
for the ComPASS collaboration



# Accelerators for America's Future

**Particle accelerators enable discovery in basic research and applied sciences**

- Probing fundamental laws of nature, discovering new particles
- Studying properties of nuclear matter
- Studying structure of crystals, amorphous materials, and organic matter
- Enhancing quality of life: medical treatment, nuclear waste transmutation, industrial applications



***Numerical modeling and simulation are essential for the development of new acceleration concepts and technologies and for machine design, optimization and successful operation***

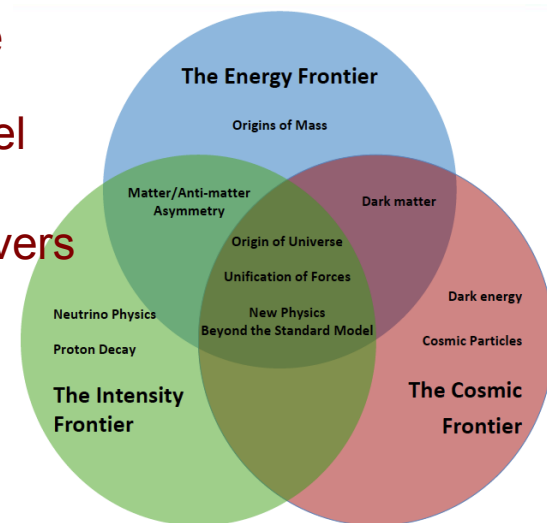


# Accelerators for High Energy Physics

- At the Energy Frontier, high-energy particle beam collisions seek to uncover new phenomena
  - the origin of mass, the nature of dark matter, extra dimensions of space.
- At the Intensity Frontier, high-flux beams enable exploration of
  - neutrino interactions, to answer questions about the origins of the universe, matter-antimatter asymmetry, force unification.
  - rare processes, to open a doorway to realms to ultra-high energies, close to the unification scale
- Particle accelerators indirectly support the cosmic frontier by providing measurements of relevant physics processes

The 2014 Particle Physics Project Prioritization Panel report identified

- 5 Science Drivers
- Mapped to 3 Frontiers



Higgs

Neutrinos

Dark Matter

Dark Energy / CMB

New particles

Energy Frontier

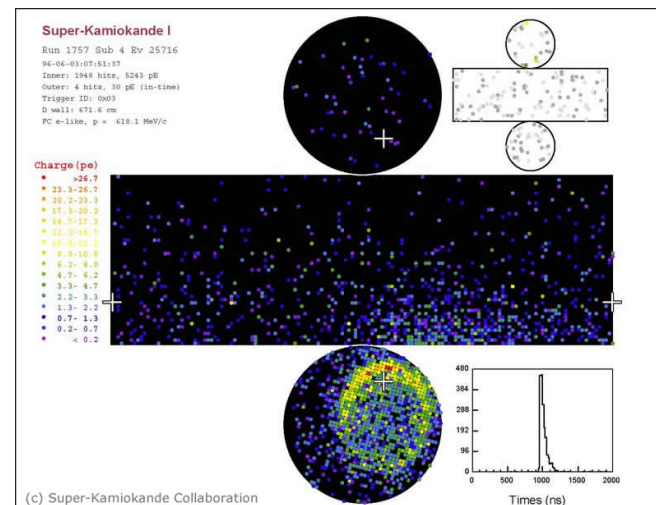
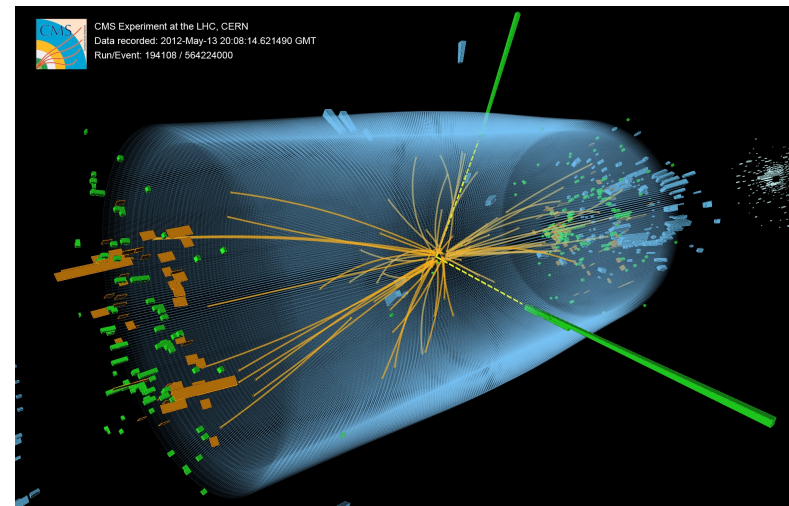
Intensity Frontier

Cosmic Frontier



# Where we are today

- Discovery of the Higgs particle, responsible for electroweak symmetry breaking and the mass of elementary particles
  - No physics beyond the “Standard Model” (SM) of HEP has been observed
- Neutrinos oscillate, thus have mass
  - No answers on mass hierarchy or symmetry properties

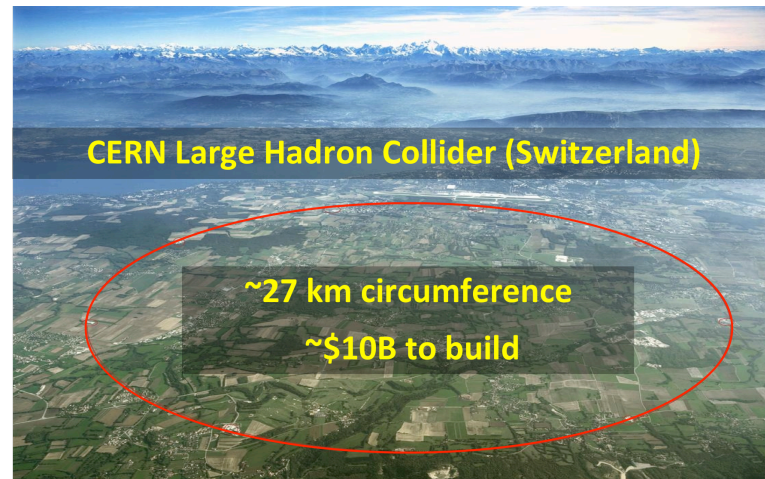


(c) Super-Kamiokande Collaboration

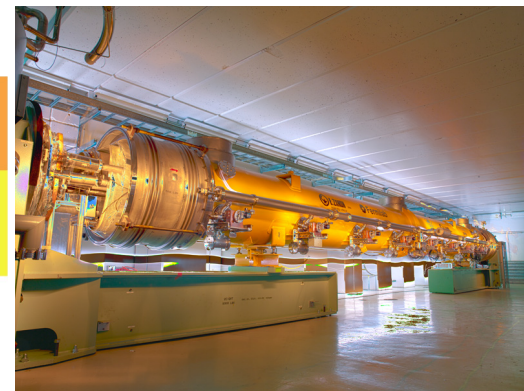
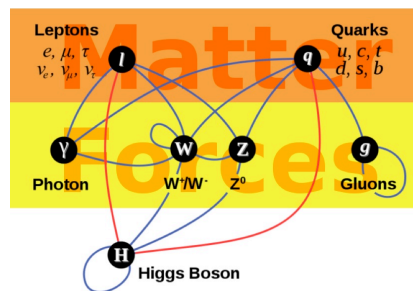


# Where we would like to be (Energy Frontier)

- A dedicated accelerator to study Higgs properties
  - “Higgs Factory” candidate: lepton collider
- More powerful accelerators to facilitate discovery
  - LHC upgrades, a new larger hadron collider
- Great accelerator science challenges!
  - Develop cost effective techniques, technologies and materials for higher acceleration gradients and more powerful magnets
  - Optimize existing technologies
    - Superconducting rf cavities, ...
  - Develop and test new accelerator designs



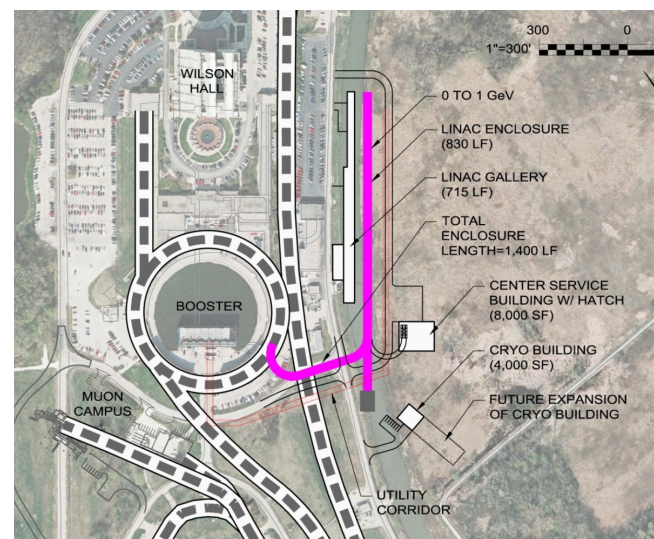
Courtesy S. Myers (IPAC 2012)





# Where we would like to be (Intensity Frontier)

- A high-intensity proton accelerator to drive
  - neutrino oscillation experiments
    - Mass hierarchy, matter-antimatter asymmetry, oscillation parameters
  - rare process experiments
    - New particles and interactions
- Staged approach at Fermilab
  - Major complex improvements Proton Improvement Plan (PIP)
  - New accelerators (PIP-II)
- A great challenge for accelerator science!
  - Minimizing and mitigating beam losses is essential
    - Instabilities from self-fields and wakefields; interplay with accelerator lattice dynamics



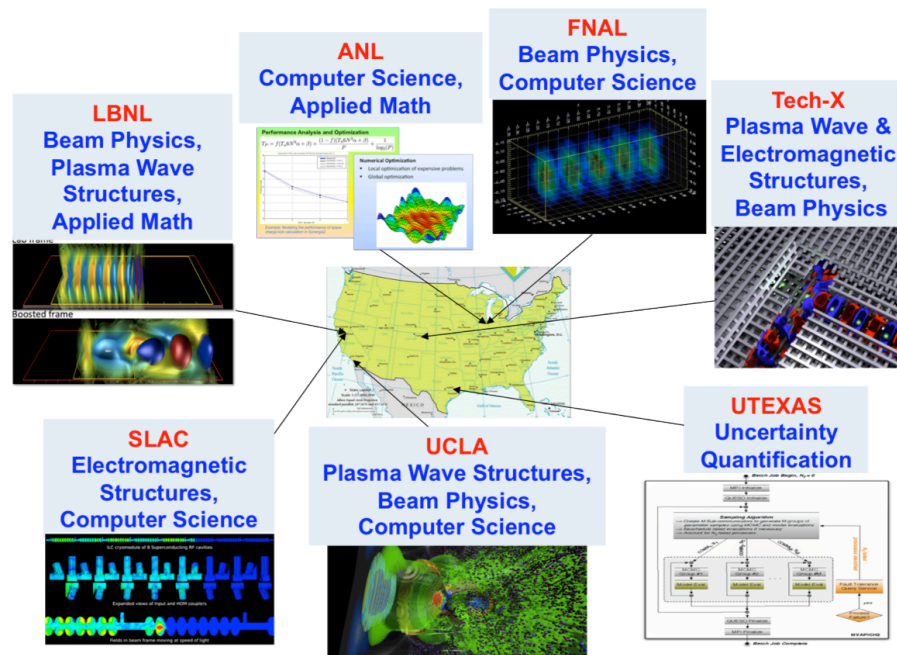


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# Advanced Computation for HEP Accelerator Science and Technology

- To enable these HEP scientific discoveries, high-fidelity simulations are required for new particle accelerator designs, concepts and technologies
- Under SciDAC3, ComPASS is developing and deploying state-of-the-art accelerator modeling tools through
  - evolution of numerical algorithms on the latest most powerful supercomputers
  - utilization of cutting-edge non-linear parameter optimization and uncertainty quantification methods.

## The ComPASS collaboration

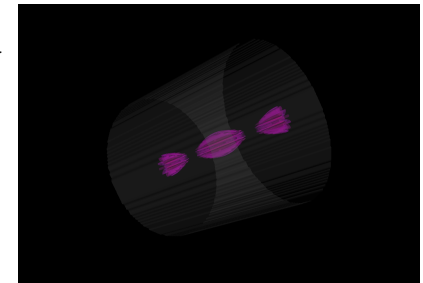
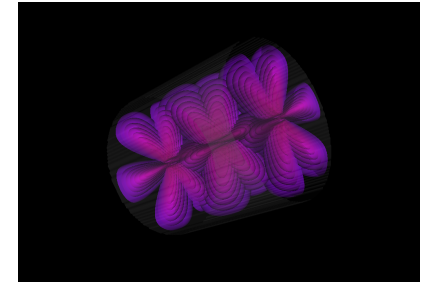


Community Project for Accelerator  
Science and Simulation (ComPASS)



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# Accelerator numerical models span a wide range of physics and scales



- Wide range of scales:
  - accelerator complex ( $10^3\text{m}$ )  $\rightarrow$  EM wavelength ( $10^2\text{-}10\text{ m}$ )  $\rightarrow$  component ( $10\text{-}1\text{ m}$ )  $\rightarrow$  particle bunch ( $10^{-3}\text{ m}$ )  $\rightarrow$  beam in plasma wakefields ( $10^{-8}$ )
- Advancing accelerator science requires development of a wide range of mathematical models and numerical algorithms!



# ComPASS Methods and Tools

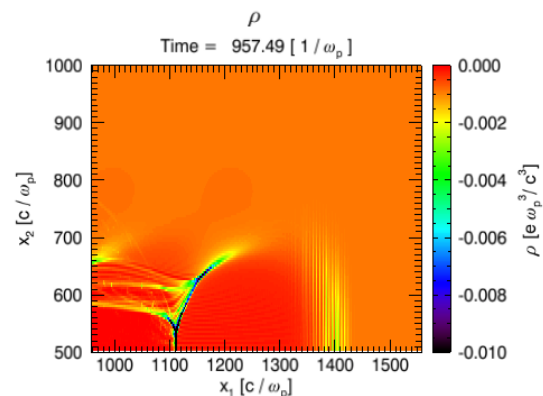
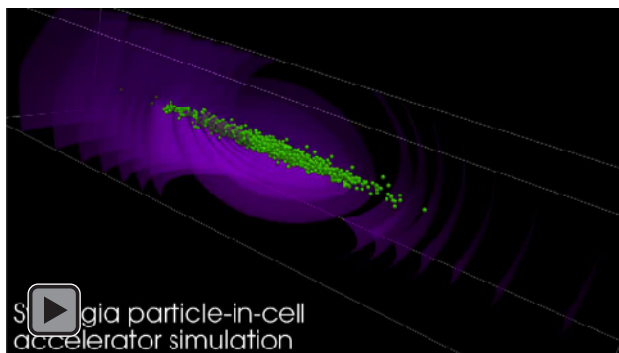
- We are developing a comprehensive set of codes that incorporate state-of-the-art field solvers
  - Electrostatic: multigrid (*Synergia*, *Warp-FastMATH*); AMR multigrid (*Warp-FastMATH*)
  - Electrostatic: spectral (*Synergia*)
  - Electromagnetic: finite element direct and hybrid (*ACE3P-FastMATH*)
  - Electromagnetic: extended stencil finite-difference (*Osiris*, *Vorpal*, *Warp-FastTMATH*); AMR finite-difference (*Warp-FastMATH*)
  - Quasi-static: spectral (*QuickPIC*)
- Collaboration with SciDAC Institutes
  - **FastMATH**: Particle in Cell techniques, field solvers (Chombo); linear algebra solvers (SuperLU) and eigensolvers
  - **QUEST**: statistical calibrations and quantitative ranking of models for plasma applications (QUESO)
  - **SDAV**: visualization (ParaView, VisIt), indexing (FastBit); domain customized applications\*
  - **SUPER**: performance analysis & optimization, non-linear parameter optimization.

**ComPASS toolkit: ACE3P, Osiris, QuickPIC, Synergia, Vorpal, Warp**



# ComPASS codes

- Six different *frameworks* developed under ComPASS
    - three focus areas: modeling of accelerator structures, beam dynamics and plasmas.
  - Although they share low-level numerical algorithm needs, the physics, problem description and numerical optimization have different requirements.
  - Beam Dynamics focus
    - Internal + External fields
      - External field calculations trivially parallelizable
      - Internal field calculations same as plasma
      - Interplay between external field dynamics and self-fields, wakes, ...
    - Minimal bunch/field structure
  - Plasma focus
    - Pure PIC
    - Complicated bunch/field structure
    - No external fields/dynamics
- Different numerical optimization and optimal numerical approaches





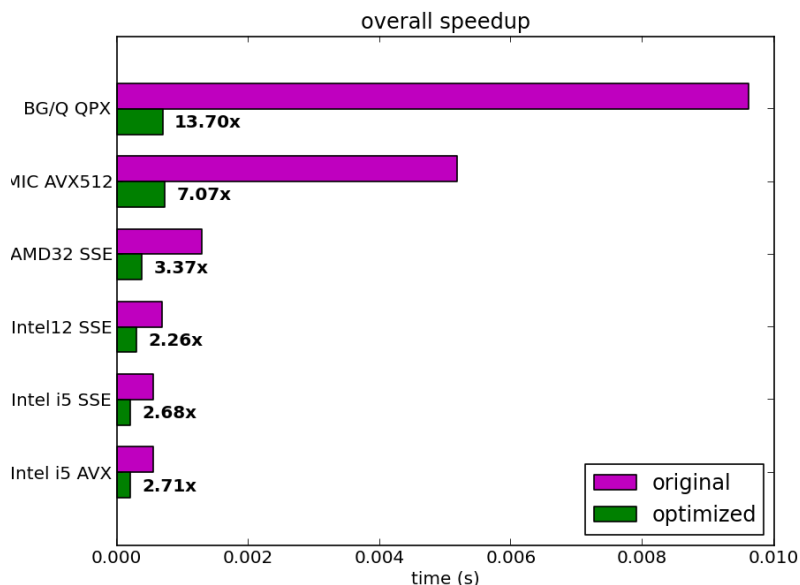
# Evolution of ComPASS tools under SciDAC3

- Enabled by our partnerships with computer scientists and applied mathematicians, ComPASS codes have
  - improved parallelism both at the MPI and node level, better data partitioning
    - allowing realistic multi-physics, multi-scale simulations
  - employed new techniques and algorithms
    - allowing modeling of previously computationally prohibitive problems
  - developed algorithms and computational framework infrastructure on modern architectures (CUDA-GPU, Intel MIC)



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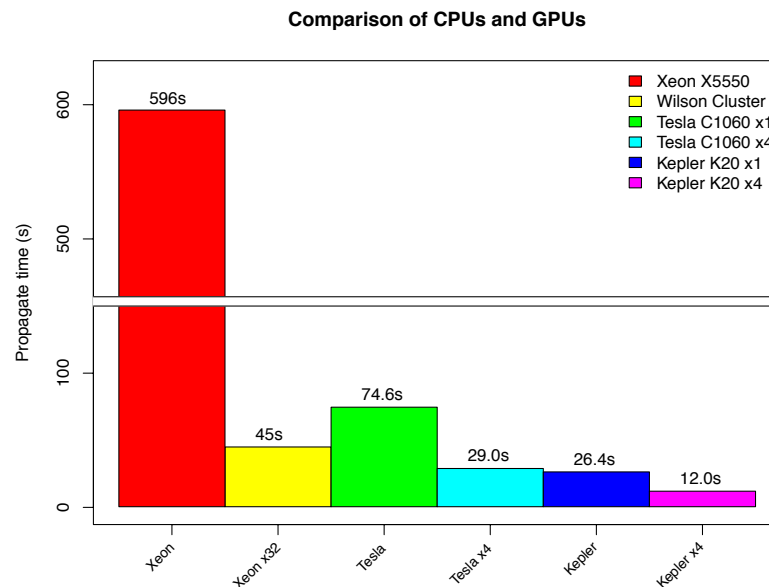
# Synergia is ported and optimized on GPU (CUDA) and MIC



*GPU-enhanced Synergia achieves better overall performance with 4 GPUs than an 128 node Linux cluster*

**First production Synergia runs on the GPU: Mu2e extraction**

*Explicit vectorization of Synergia single-particle routines leads to a large performance enhancement across architectures*

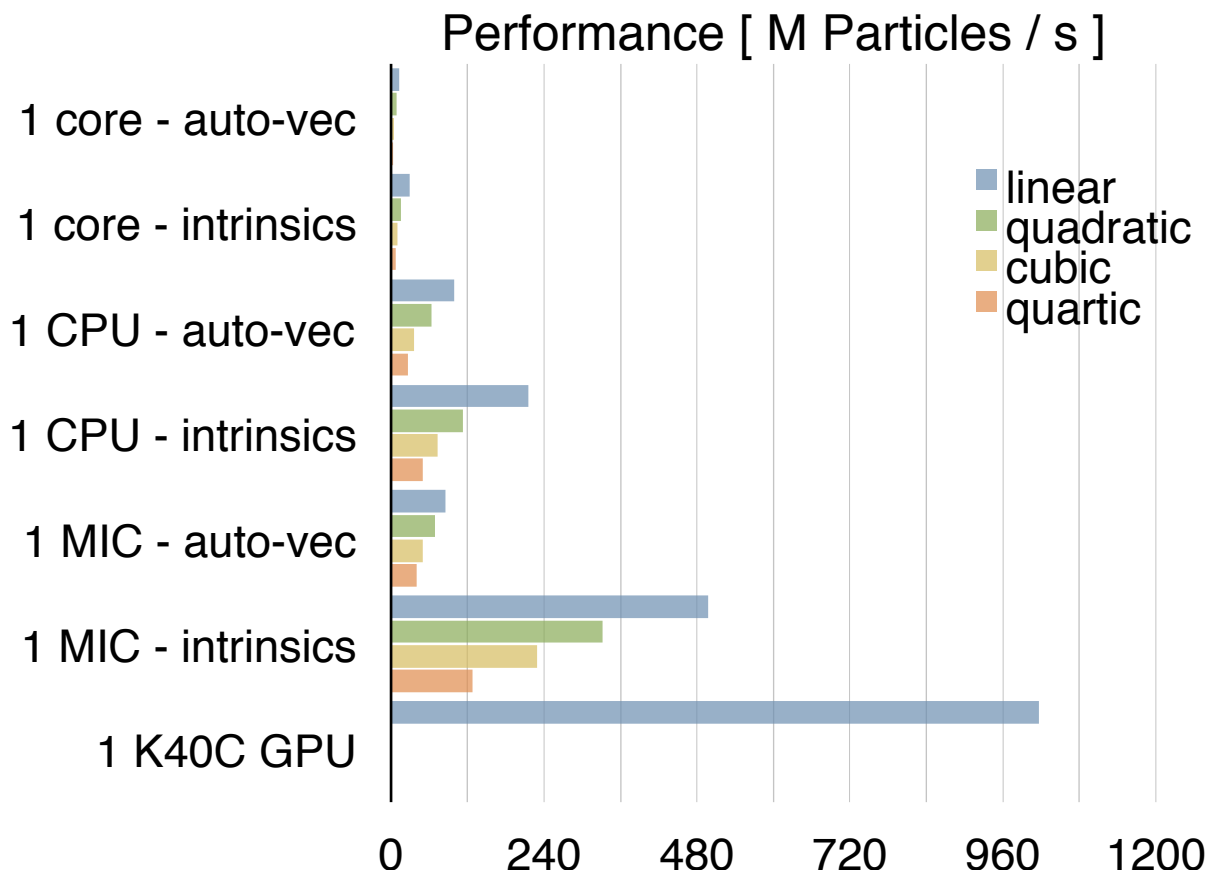


ASCR funded work at FNAL, Qiming Lu, James Amundson



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# OSIRIS is ported on GPU (CUDA) and Intel Phi



Explicit vectorization also plays a key role in CPU / core

Combining the 8 cores in the CPU yields over 200 M Particle pushes per second

Using automatic vectorization gives approximately the same performance for 1 MIC as for 1 CPU auto

Explicit vectorization gives a significant boost from CPU version

OSIRIS runs across clusters of accelerators

*ASCR funded work  
at UCLA*

V.K. Decyk, R.A. Fonseca, A. Tableman



# ComPASS SciDAC3 applications

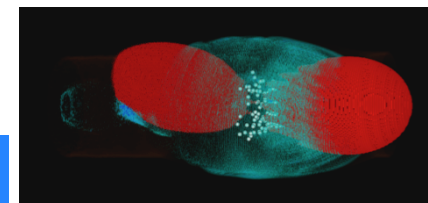
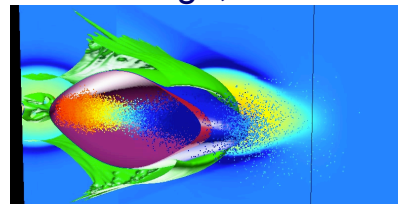
- Support the development and study of new technologies for smaller and possibly cheaper energy frontier accelerators:
  - accelerators based on standard technology are limited by the metallic electrical breakdown limit of 50-100 MV/m
  - plasma based acceleration: a driver beam (laser/particles) propagating through a plasma creates a wake with accelerating gradients exceeding 50 GV/m.
  - dielectric laser accelerators: a laser propagating through a dielectric lattice can generate electric fields of few GV/m
- Support optimization and upgrades of conventional technology accelerators
- Support the design and optimization of high-intensity proton accelerators to minimize beam losses that cause radiation damage. Modeling of
  - many (all) beam bunches in circular machines and their coupling through impedance and wakefields
  - beam self-charge and instabilities caused by beam-matter interactions
  - field non-linearities and accelerator geometry
- Focus on the Fermilab Proton Improvement Plan (PIP)



# Energy Frontier Applications

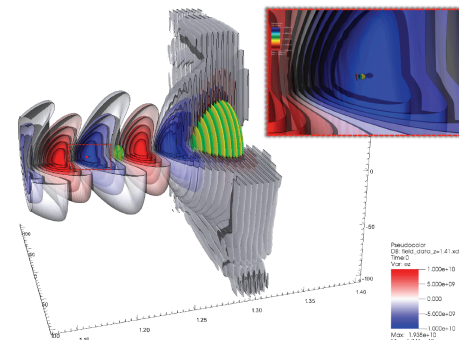
- Plasma-based acceleration:
  - support the BELLA (laser) and FACET (beam) experimental programs
  - develop techniques to improve beam quality
  - study controlled electron beam injection
  - improve staging for future lepton collider concepts.
- Dielectric laser acceleration:
  - design efficient power couplers between optical fiber and accelerator structure
  - explore wakefield effects and associated break-ups for different topologies
  - design structures able to accelerate high quality beams
- LHC upgrade:
  - ComPASS tools used for the design of the LHC Injector upgrade

FACET stage, QuickPIC

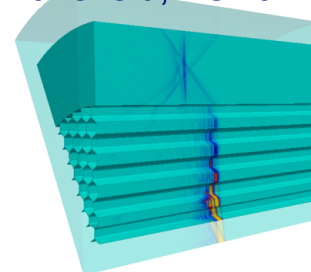


Colliding pulse injection,  
Vorpal

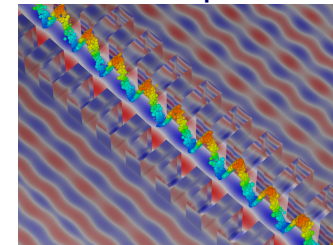
2-color  
injection,  
WARP



PBG wakefield, ACE3P



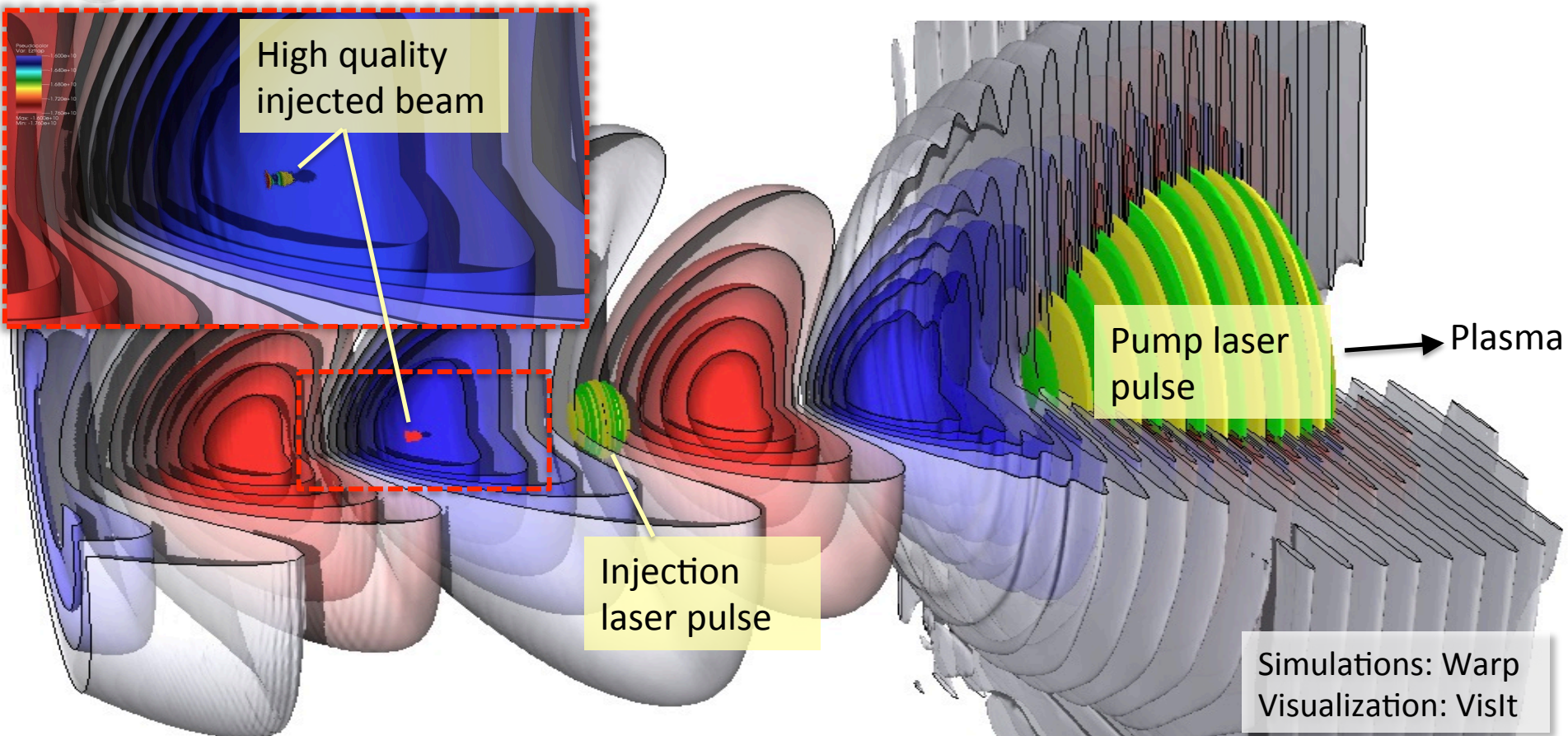
Dielectric grating structure  
Vorpal





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# Large scale 3-D simulations validate a new concept for injection of very high-quality beams\*



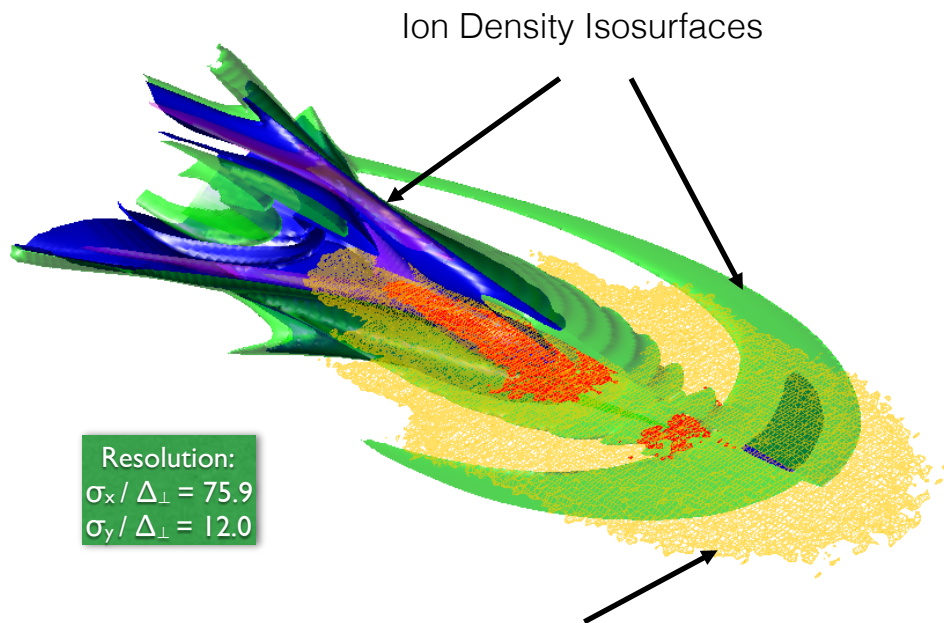
- 1 - Pump laser pulse creates accelerating wake in plasma.
- 2 - Injection laser ionizes pocket of Krypton gas, creating very high-quality electron beam.
- 3 - Electron beam is accelerated to high energy in short distance by wake.

Parametric runs necessitated over a million hours; typical 3-D run around 100k core-hours.

\*L.-L. Yu, E. Esarey, C. B. Schroeder, J.-L. Vay, C. Benedetti, C. G. R. Geddes, M. Chen, and W. P. Leemans, *Phys. Rev. Lett.* **112**, 125001 (2014)



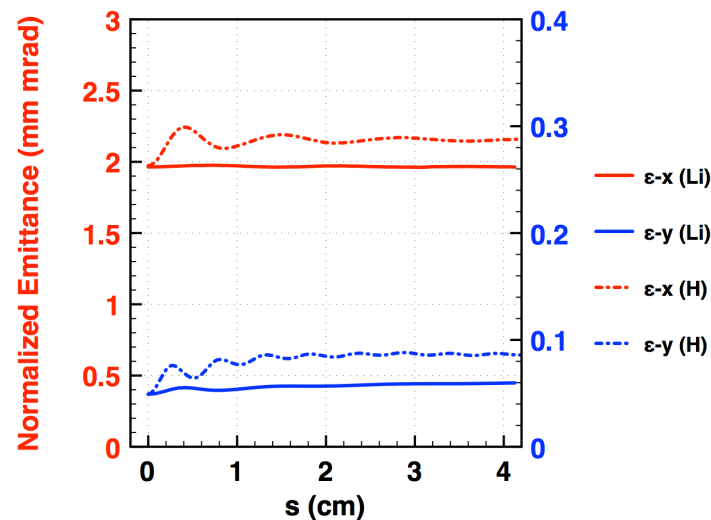
## Density Isosurfaces of the Ion Collapse in a Hydrogen Plasma



Electron Beam with Asymmetric Spot Size

Trailing Beam:  $\sigma_z = 10.0 \mu\text{m}$ ,  $N = 1.0 \times 10^{10}$ ,  
 $\sigma_x = 0.463 \mu\text{m}$ ,  $\epsilon_{Nx} = \mathbf{2.0 \text{ mm}\cdot\text{mrad}}$ ,  
 $\sigma_y = 0.0733 \mu\text{m}$ ,  $\epsilon_{Ny} = \mathbf{0.05 \text{ mm}\cdot\text{mrad}}$   
 $\mathbf{Y = 48923.7 (25 \text{ GeV})}$ , Plasma Density:  $1.0 \times 10^{17} \text{ cm}^{-3}$

Beam Emittance



**In Li, the emittance in x does not change, and in y direction it only increase by 20%.**

**In H, the emittance in x increase by 10%, and in y direction it increases by 70%.**

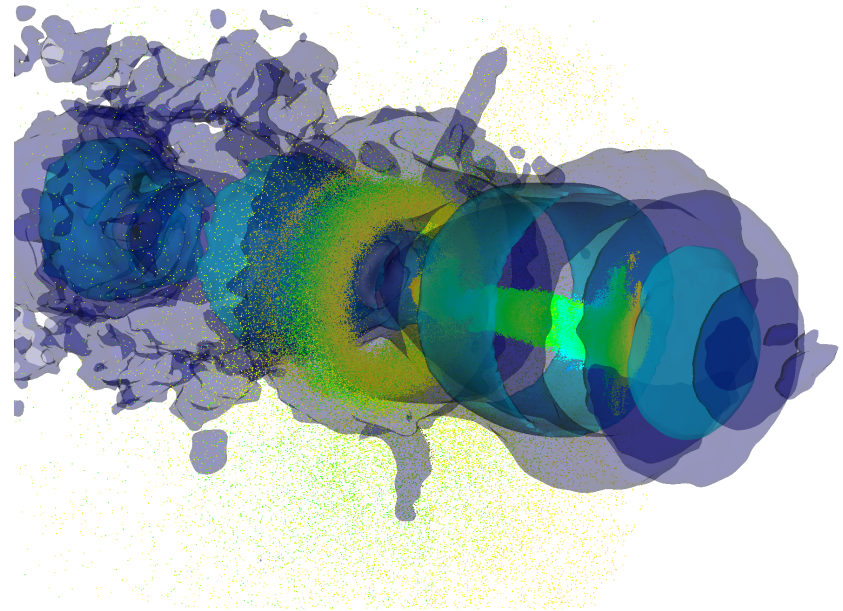
This study required QuickPIC runs with 16384 x 16384 x 2048 cells on 32768 processors

W. An et al.



# Large scale simulations explain electron beam ring formation in LWFA experiments

- LWFA experiments at LLNL show, a monoenergetic electron ring feature. 3D OSIRIS simulations were performed to understand the underlying physics. They identify that laser evolution in the experiments is responsible for the formation of the ring feature.
- Simulation Parameters:
  - 300 x 300 x 4000 grids, ~5 billion particles, ~500,000 time steps
  - A few 1.5 million core hour simulations were performed.

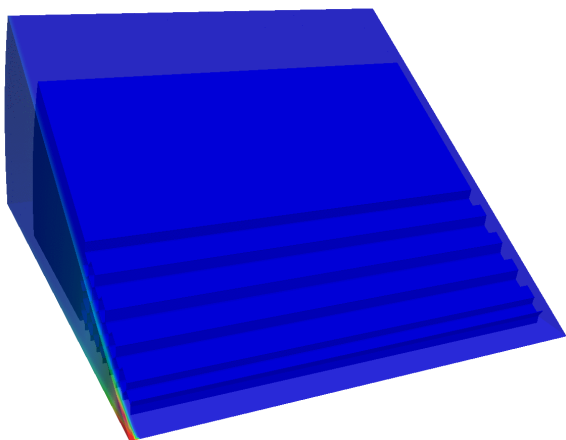
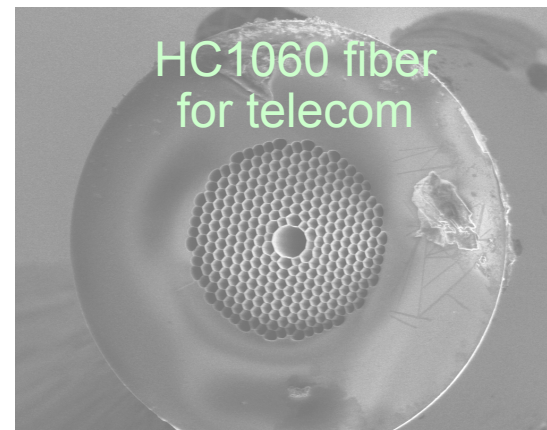


F.S. Tsung et al.

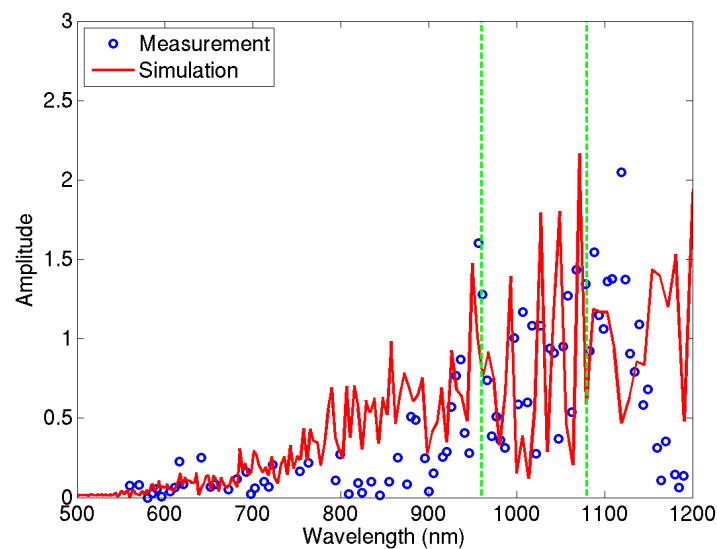


# Wakefield in Photonic Bandgap Fiber for Dielectric Laser Acceleration

- Simulation model is built based on fiber SEM images.
- The radiated spectrum from beam-driven simulation agrees fairly well with spectrograph measurements at NLCTA test facility at SLAC.
- The existence of bandgap modes in the PBG fiber has been demonstrated through experiments and simulations.
- ACE3P simulation was done in several hours using 14k cores on hopper.



Beam transit in PBG fiber using ACE3P



Comparison of simulation and measurement



# Synergia for CERN LHC Injectors Upgrade (LIU)

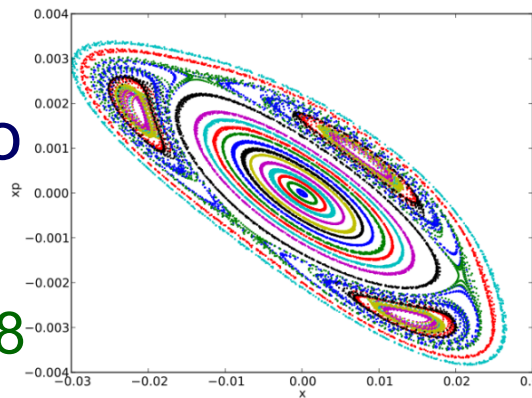
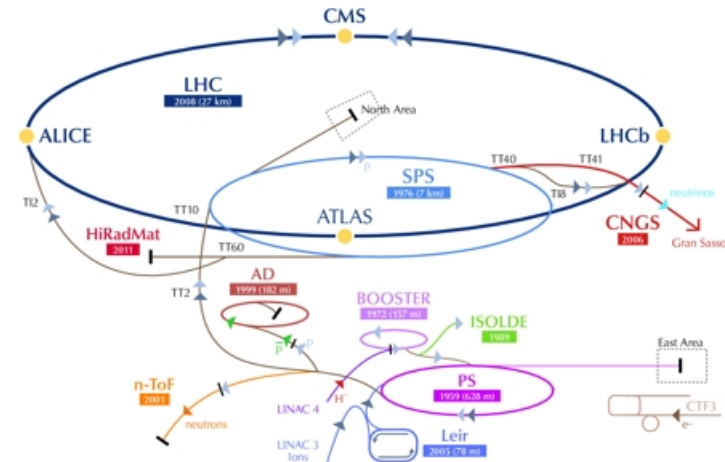
- The US is investing ~1B\$ for the LHC upgrades

- CERN LIU project aims to deliver the intense and reliable input beams required by the High Luminosity LHC

- Detailed modeling of intensity-dependent effects is crucial for success

- Work in collaboration with CERN scientists to utilize Synergia

- Massive simulations to validate using GSI SIS18 ring data



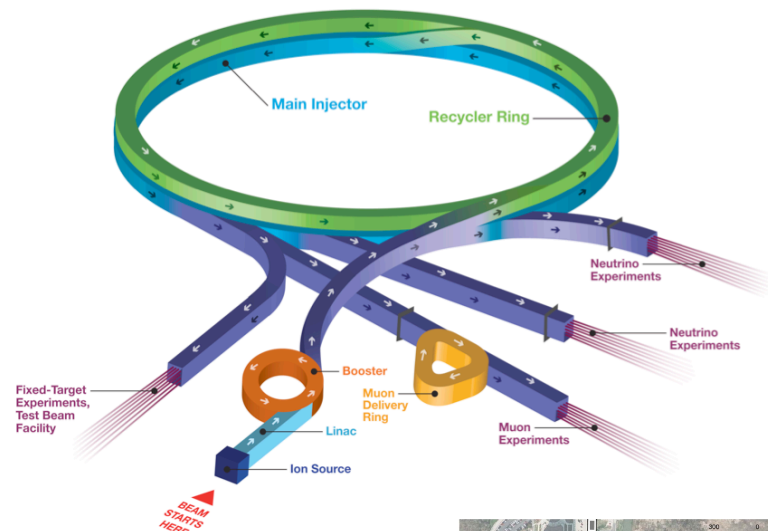
- 71 steps/turn
- 100k turns
- 7,100,000 steps
- 4,194,304 particles
- 29,779,558,400,000 particle-steps
- 1,238,158,540,800,000 propagator calls



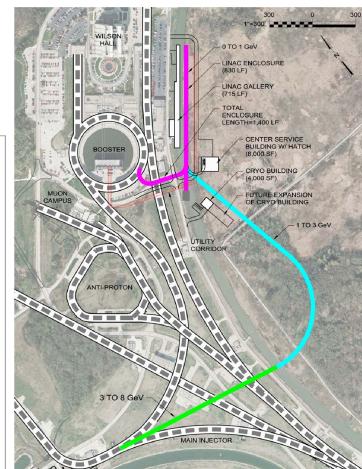
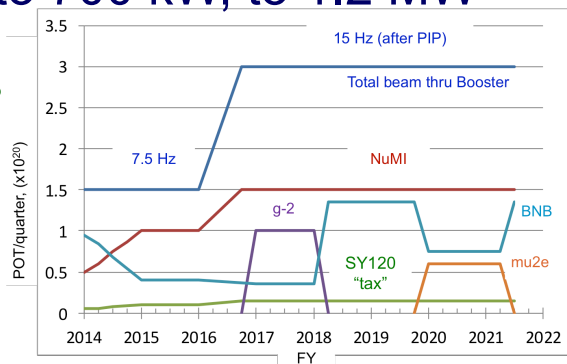
# Intensity Frontier Applications

- Fermilab proton source upgrades for the Neutrino and Muon Programs (PIP)
  - Booster synchrotron: instability control for beam quality and loss minimization
  - Main Injector (MI) and Recycler: instability mitigation and loss minimization
- Mu2e upgrades
  - Optimize Delivery Ring extraction design
- New srf Linac (PIP-II)
  - Linac design: study wakefields
  - MI operation: study electron-cloud effects and beam loss mitigation techniques

Fermilab Accelerator Complex



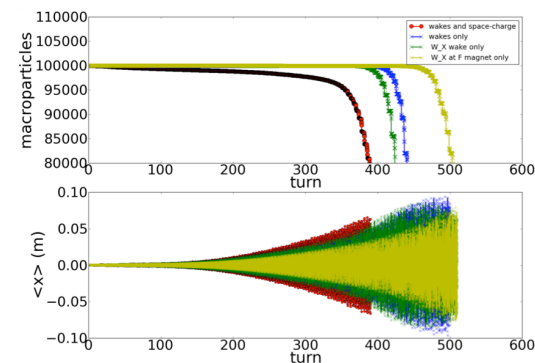
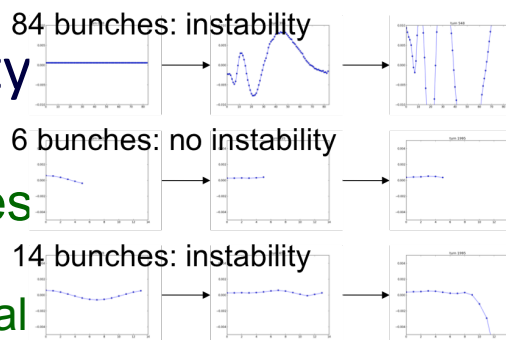
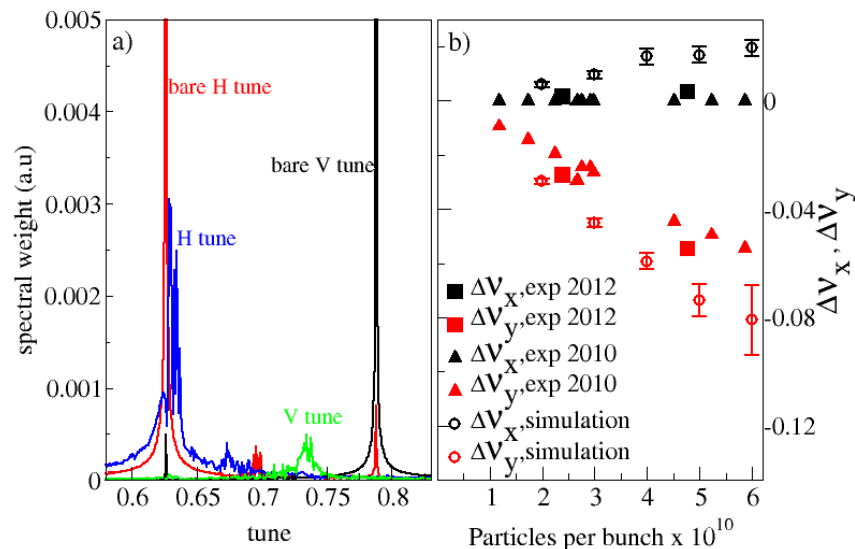
Power increase from 300 to 700 kW, to 1.2 MW





# Booster PIP

- Horizontal plane coherent instability observed near injection
  - Problem solved by empirically modifying chromaticity, at a counterintuitive value
- Large-scale Synergia multi-bunch simulations revealed the precise source of a wakefield-initiated instability
  - accurately describe all relevant measured quantities
    - model can now provide guidance to determine optimal operational parameters

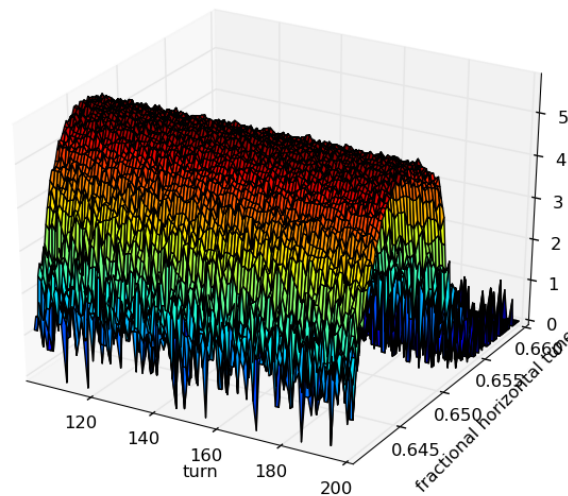
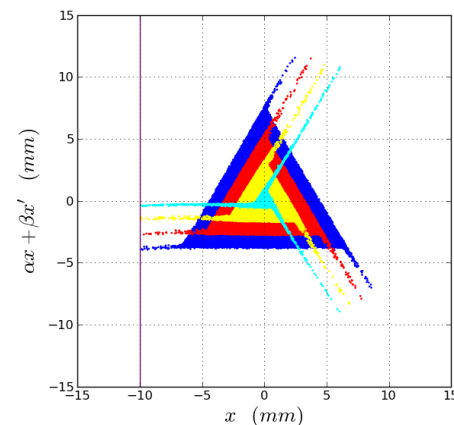
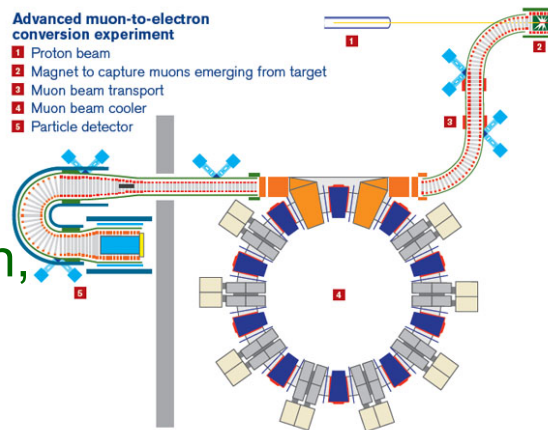


A. Macridin, et al., PRST-AB 16, 121001 (2013)



# Intensity Frontier: Mu2e extraction design

- Synergia full extraction simulation for the Muon to Electron (Mu2e) experiment
  - 26k turns, 240 3D solves/turn, 1M macroparticles
  - include apertures and non-linear fields (external)
  - Quantitative beam loss predictions
- Optimization campaign determines ramping profile that maximizes beam uniformity
  - Essential to minimize physics signal background

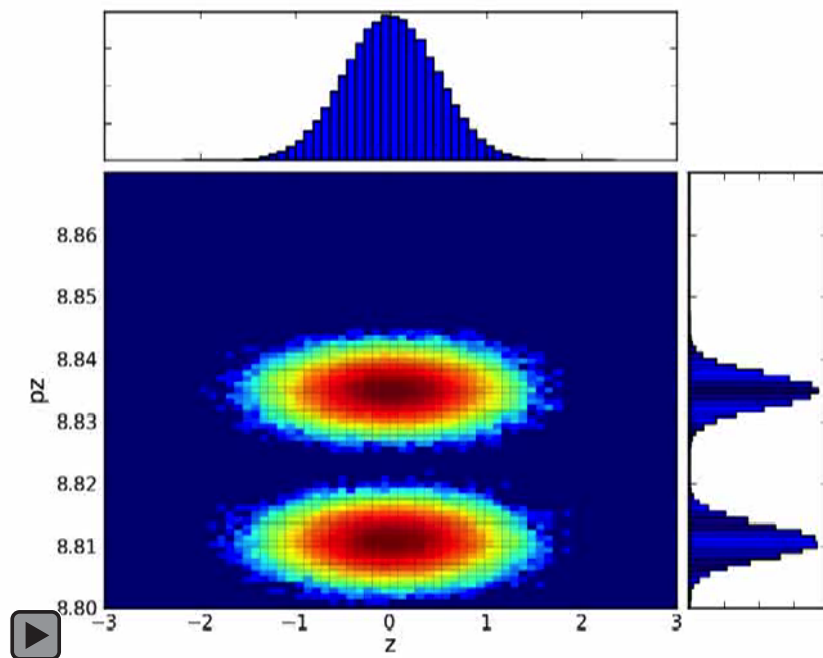


C.S. Park et al, results contributed to the Critical Decision process for the experiment



# Recycler slip-stacking

- Slip stacking of Booster bunches used to increase intensity in the MI
  - In the past, done directly in the MI
- Under PIP, to increase the MI ramp rate (thus beam power) process moved to the Recycler
  - Essential to model the whole process, characterize localized losses and evaluate mitigation techniques
  - A very complex model simulation campaign underway





# Synergia Simulation campaign for PIP

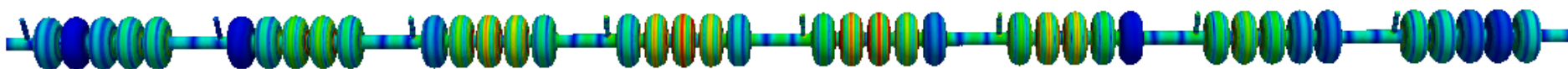
- Single job size for production
  - Booster 20k core
  - MI/Recycler 64 k core
  - Parameter scans for optimization 131k core
- For the results presented here, the simulation campaign used 80M core hours at the ALCF, on Intrepid and Mira



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# ACE3P Simulation of PIP2 Cryomodule

- A scalable hybrid linear solver PDSLIn (LBNL/FASTMath) with improved memory usage compared with direct solver in **Omega3P** advances large-scale cavity mode calculation.
- Solution time is substantially reduced. It took 3 min to calculate a mode frequency and its damping using 300 cores, 1.1 Tbytes of memory for a mesh with 14M degrees of freedom on NERSC Edison supercomputer.



A trapped monopole mode (2.413 GHz) in Fermilab PIP2 650 MHz cryomodule consisting of 8 SRF cavities

# Awards given to novel methods developed partially under SciDAC-ComPASS 2 & 3



Jean-Luc Vay awarded:

- **2013 US Particle Accelerator School Prize** for Achievement in Accelerator Physics & Technology  
*“For original contributions to the development of novel methods for simulating particle beams, particularly the **Lorentz boosted frame** techniques, and for the successful application of these methods to multi-scale, multi-species problems.”*
- **2014 NERSC Achievement Award** in Innovative use of High Performance Computing  
*“For developing innovative tools for multi-scale simulations of beams and plasmas (more specifically the work on **boosted frame** and **novel spectral decomposition techniques**).”*

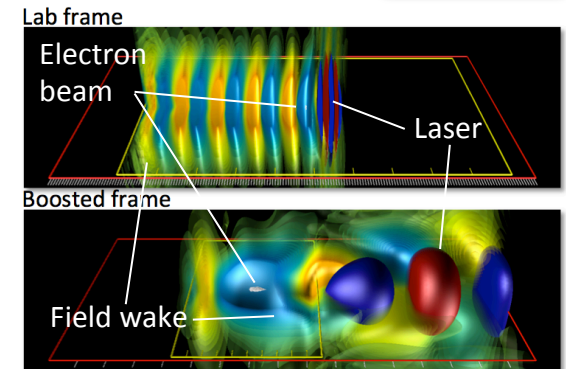
## Lorentz boosted frame approach

uses special relativity to speed-up calculation by orders of magnitude



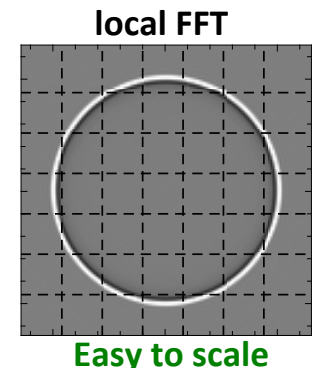
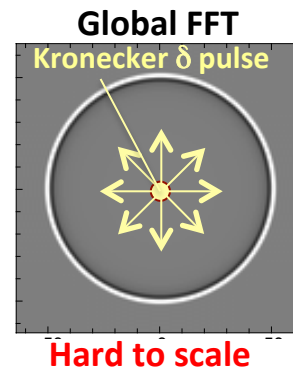
Laser-plasma Accelerators

Max speedup demonstrate  $d > 1$  million



## Novel spectral parallel decomposition paradigm

uses finite speed of light to replace global FFTs by local FFTs in spectral electromagnetic solvers





# Summary

- Particle Accelerators are the most important instruments of discovery in HEP
  - in addition, they have many quality-of-life-enhancing applied science and industrial applications outside HEP
- Numerical modeling and simulation are essential for the development of new concepts and technologies and design and operation optimization
  - because of the complexity and many scales involved HPC is required for model fidelity
- ComPASS under SciDAC3 is developing and deploying state-of-the-art HPC accelerator modeling tools
  - major collaboration (and opportunity for) with SciDAC institutes
  - already mature tools are supporting major activities of the accelerator community